

Claims

1-4. (canceled).

5. (currently amended). A computer-implemented method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing, and wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation;

producing fixed bond information based on the selection; and

outputting the fixed bond information.

6. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes a ring system with a hetero substitution pattern.

7. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes a non-cyclic system.

8. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes an acyclic system.

9. (currently amended). A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;
selecting from among the plurality of fixed bond representation candidates based on the evaluation;
producing fixed bond information based on the selection;
based on the fixed bond information, producing a fixed bond representation that includes a pair of opposite charges lacked by the delocalized representation; and
outputting the fixed bond representation.

10. (currently amended). A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing;
identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
evaluating at least a subset of the fixed bond representation candidates;
selecting from among the plurality of fixed bond representation candidates based on the evaluation;
producing fixed bond information based on the selection;
based on the fixed bond information, producing a fixed bond representation that includes a pair of radicals lacked by the delocalized representation; and
outputting the fixed bond representation.

11. (previously presented). The method of claim 5, wherein the step of identifying is performed based on electronic state and valence distribution (ESVD), and further comprising: queuing at least a subset of the ESVDs by priority.

12. (currently amended). A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation;

producing fixed bond information based on the selection;

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the delocalized representation; and

outputting the fixed bond information.

13. (previously presented). The method of claim 12, wherein the table is configured to allow additional elements and values to be added.

14. (previously presented). The method of claim 12, wherein the table is configured to allow additional elements and values to be added to apply to any chemical element.

15. (previously presented). The method of claim 5, further comprising:
deriving electronic state and valence distributions information together with analyzing the delocalized representation.

16. (previously presented). The method of claim 5, further comprising:
determining, by either exhaustion or exceeding a predetermined amount of time, whether it is possible to produce a neutral, non-radical fixed bond representation of most chemical structures.

17 and 18. (canceled).

19. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes a monocyclic ring system.

20. (currently amended). A computer-implemented system for use in deriving fixed bond information, comprising:

an analyzer analyzing a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing, and wherein at least a portion of the delocalized representation describes a polycyclic ring system;

an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates;

a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and

a producer producing fixed bond information based on the selection;

said fixed bond information being output by the system.

21. (currently amended). Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing, and wherein at least a portion of the delocalized representation describes a polycyclic ring system;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates;

select from among the plurality of fixed bond representation candidates based on the evaluation;

produce fixed bond information based on the selection; and

outputting the fixed bond information.

22. (new). The method of claim 5 wherein the step of identifying includes tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected.

23. (new). The method of claim 9 wherein the step of identifying includes tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected.

24. (new). The method of claim 10 wherein the step of identifying includes tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected.

25. (new). The method of claim 12 wherein the step of identifying includes tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected.

26. (new). The system of claim 20 wherein said identifier traces a path through the structure, assigns bond orders and atomic charges/radicals as the path is traced, and backtracks the path when an inconsistency is detected.

27. (new). The computer software of claim 21 wherein the instructions for causing the system to identify, include instructions for tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected.